



**German Chemical Society
Gesellschaft Deutscher Chemiker**

GDCh-Advisory Committee
on Existing Chemicals of
Environmental Relevance (BUA)

**1-Chloro-2-methyl-3-nitrobenzene
(2-Chloro-6-nitrotoluene)**

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(March 1991)



S. Hirzel

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Beratergremium für
Umweltrelevante Altstoffe (BUA)



S. Hirzel

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Foreword

The German Chemicals Act (Chemikaliengesetz - ChemG) of 1980 stipulates that certain existing chemicals must be reported to the competent authority, if they exhibit properties which indicate that they may be hazardous, either alone or in combination with other substances.

In the summer of 1982, an Advisory Committee on Existing Chemicals of Environmental Relevance (BUA) was set up by the German Chemical Society (Gesellschaft Deutscher Chemiker - GDCh). It brings together representatives from the scientific community, the chemical industry and the governmental authorities. This Advisory Committee is responsible for elaborating appropriate solutions for substances of relevance for health and the environment on the basis of voluntary measures. It selects and examines existing chemicals from the aforementioned angles. The testing and evaluation are based on scientific criteria alone.

It was, therefore, necessary to develop priority setting procedures. In a first phase reports were only prepared for priority chemicals. Within the framework of a first priority setting procedure, chemicals were compiled from several priority lists and 135 chemicals were selected for detailed substance reports.

In a second priority setting procedure the survey of the German Chemical Industry Association (VCI) on all substances with a production volume of more than 10 tons per year was used as a starting list. Since this survey covered 4,600 chemicals, BUA decided to process the corresponding list in several stages. The first stage included approx. 1,050 substances with a production volume of more than 1,000 tons per year.

Detailed reports are drawn up on chemicals suspected of having a hazard potential and abridged reports on those presenting only a minor hazard potential, according to the current state of knowledge.

The detailed BUA reports take in both the published literature and data from industry. If data for the evaluation of the chemicals are not available, additional studies are recommended and the results are published as updates to the reports. The reports serve as a basis for the instigation of administrative measures, when there are indications of risks to health or the environment.

Tübingen, May 1993

Ernst Bayer
Chairman of the Advisory Committee
on Existing Chemicals
of Environmental Relevance

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(2-Chloro-6-nitrotoluene)

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BUA Report on 1-Chloro-2-methyl-3-nitrobenzene

(2-Chloro-6-nitrotoluene)

Summary and conclusions

Ecological aspects

Occurrence and partitioning in the compartments

In the Federal Republic of Germany (within the frontiers of September 1990) 1-chloro-2-methyl-3-nitrobenzene, synonym 2-chloro-6-nitrotoluene, was manufactured in 1990 in a quantity of 500 t and processed by hydrogenation to 3-chloro-2-methyl-aniline (3-chloro-*o*-toluidine) as the only direct consequential product; the latter is an initial product for dyes and pigments, pharmaceuticals and pesticides.

The discharge into the environment from industrial production and processing takes place via waste water and to a minor extent via vent air. The discharge via waste water from production and processing is estimated at about 660 kg, 600 kg coming from manufacture in 1990, 60 kg from processing.

The discharge via vent air from production and processing in 1990 is estimated at 10 kg.

Within the scope of a monitoring programme, 2-chloro-6-nitrotoluene is periodically measured in the Main river downstream of the only manufacturing and processing plant in the Federal Republic of Germany, the values measured in 1984 - 1987 ranging from less than 0.05 µg/l (determination limit) to 3.0 µg/l (90-percentile 0.5 µg/l).

There is no information available on the occurrence in other surface water bodies.

2-Chloro-6-nitrotoluene could not be detected in the sediment of the lower Main river on the occasion of measurements performed in 1980.

In 1982 2-chloro-6-nitrotoluene was detected qualitatively in fish sample in the Main river, quantitative determinations of levels in the biosphere, however, are lacking.

There are no studies on the occurrence in the soil either, nor on soil sorption and motility, respectively. Because of the log P_{OW} of about 3 and other properties of 2-chloro-6-nitrotoluene, a mean soil sorption must be taken into account.

There are no measurements as to the occurrence of 2-chloro-6-nitrotoluene in the atmosphere. On the basis of a calculation according to Mackay, the partial transition of the substance from the water bodies into the atmosphere must be taken into account. Therefore, regionally limited occurrence in the atmosphere is possible.

Degradability

On a laboratory scale, 2-chloro-6-nitrotoluene can be eliminated at a rate of 80 - 90 % by treatment with adapted sewage sludge being adsorbed onto activated charcoal (modified Zahn-Wellens-test).

There are no further studies on the biodegradability.

No studies on hydrolytic degradation are available, either.

A half-life time of about 48 days has been calculated for the photo-chemical oxidative degradation by OH radicals in the atmosphere.

Bioaccumulation

According to the n-octanol/water partitioning coefficient ($\log P_{OW} = 3.09$) bioaccumulation must be taken into account.

In fish a bioconcentration factor of about 100, based on wet weight of whole fish, was determined experimentally.

Ecotoxicology

The toxicity in aerobic bacteria (EC_{10} after 30 minutes exposure) is reported as 109 mg/l for *Pseudomonas putida*. In the photobacteria test with *Photobacterium phosphoreum* an EC_{10} of 0.085 mg/l results after 30 minutes exposure.

The toxicity in algae is indicated with a 4 h EC value of 16 mg/l for *Haematococcus pluvialis*.

The acute toxicity in the Daphnia is reported by various authors as ranging between 2 and 5 mg/l, based on immobilisation after 24 hours exposure.

In the 21 days reproductive toxicity test in Daphnia, a concentration of 0.63 mg/l was determined as the NOEC; 1.25 mg/l was found as the lowest concentration influencing maternal mortality, reproduction rate and appearance of the first brood.

The 96 h LC_{50} in the golden ide was determined to 9.04 mg/l, the NOEC to 4.0 mg/l. As to the LC_{50} in the guppy after 14 days exposure, 5.2 mg/l are reported.

Toxicological aspects

2-Chloro-6-nitrotoluene is an indirect methemoglobin-forming agent. Respiratory distress, cyanosis and narcosis were observed in the rat after single oral administration.

The oral LD₅₀ is 2320 and 2560 mg/kg bodyweight, respectively, in the rat (male, female). Necropsy findings are dark discolorations of liver and adrenals, brightening areas in the liver and tracing of the hepatic lobules. An orientation test in the cat resulted in strong methemoglobin formation and an oral LD₅₀ inferior to 50 mg/kg.

No symptoms of intoxication appeared in the rat after single oral administration of 2000 mg 2-chloro-6-nitrotoluene/kg, the necropsy findings were also negative. An LD₅₀ of 56 mg/kg is reported for the single intravenous administration in mice. The inhalation hazard test was negative. Slightly irritant effects resulted from the assessment of skin and mucous membrane tolerance.

No information on sensitizing activity, on subchronic and chronic toxicity, on genotoxicity, carcinogenicity and reproductive toxicity are available.

In man appearance of cyanosis was observed after exposure to chloro-nitrotoluene isomers.

Recommendations

Ecology

Further studies on biodegradability by adapted and non-adapted microorganisms are recommended. Existing monitoring programs should be continued.

Toxicology

Data on toxicokinetics and metabolism, on subacute, subchronic and chronic toxicity, on mutagenicity, carcinogenicity and reproductive toxicity are lacking.

In view of the low exposure level of man, these investigations should be performed in order to clarify the risk of toxic effects relevant to the work place rather than with regard to environmental protection.

It is recommended to perform a micronucleus test in order to further clarify the mutagenic potential evidenced by the Ames test with metabolic activation.